Supplemental Material

Tuning the electronic properties of asymmetric YZrCOF MXene for water splitting applications: An ab initio study

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Wannierization of a band structure

Wannierization of a band structure involves obtaining maximally localized Wannier functions (MLWFs)[2] from the electronic band structure obtained through a first-principles calculation. We have constructed the MLWF (minimally localized Wave functions) basis and interpolated the obtained (KS) energies onto different mesh as shown on the Band structure plot; a converged $8 \times 8 \times 1$ grid was found, see both of Figures S1 and S2. An efficient basis of minimally localized Wannier functions must be constructed since the band structure along high symmetry lines is required. The Wannier orbitals' overall quadratic spread can be minimized to produce these. When MLWF is calculated for a particular material, the bands of interest typically form an entangled set rather than an isolated set. In this instance, a two-step technique is used: (step 1) Disentanglement: Select an appropriate energy window for building the MLWF. In our example, the maximum energy for the frozen window is dis_froz_max = -2.2313 eV (around the Fermi level), and the maximum energy for the disentanglement dis_win_max = 20 eV. (step 2) spread minimization, where the spread functional of MLWF is minimized. In our case, the outer window (the disentangle window) between -49.96 and 20 eV and the inner window (the frozen window) between -49.96 and -2.2313 eV was adjusted to have a given value disentanglement. The converged band structure along the path through the Brillouin zone using DLWFs is presented in Figure S3.

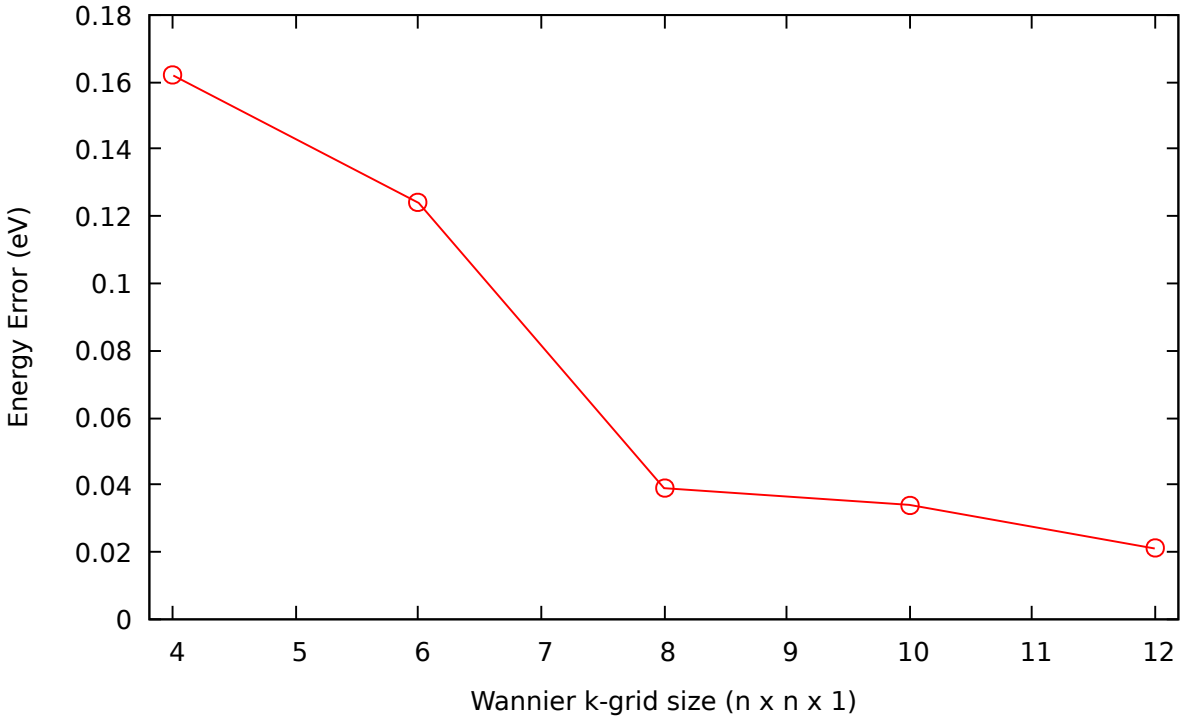

Figure S1 Maximum energy error (eV) for Wannier function made with different k-grids near Fermi level

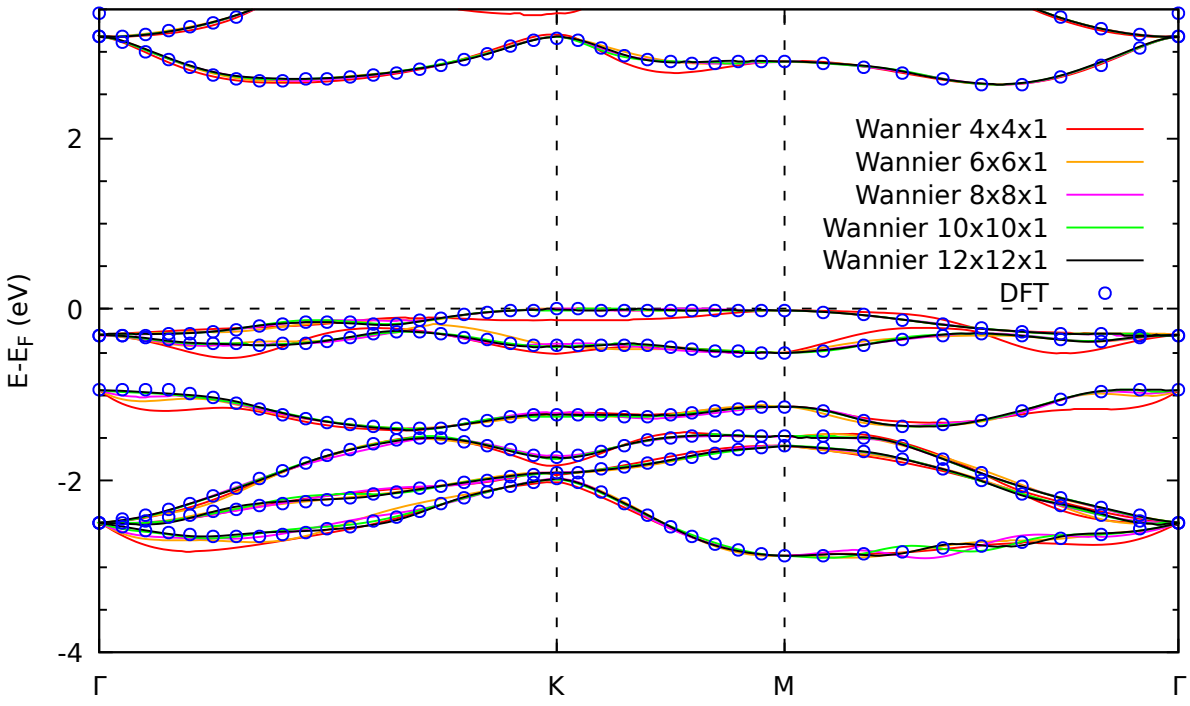

Figure S2 Comparison of DFT and Wannier band structures for YZrCOF monolayer with different Wannier k-grids along high-symmetry Brillouin zone.

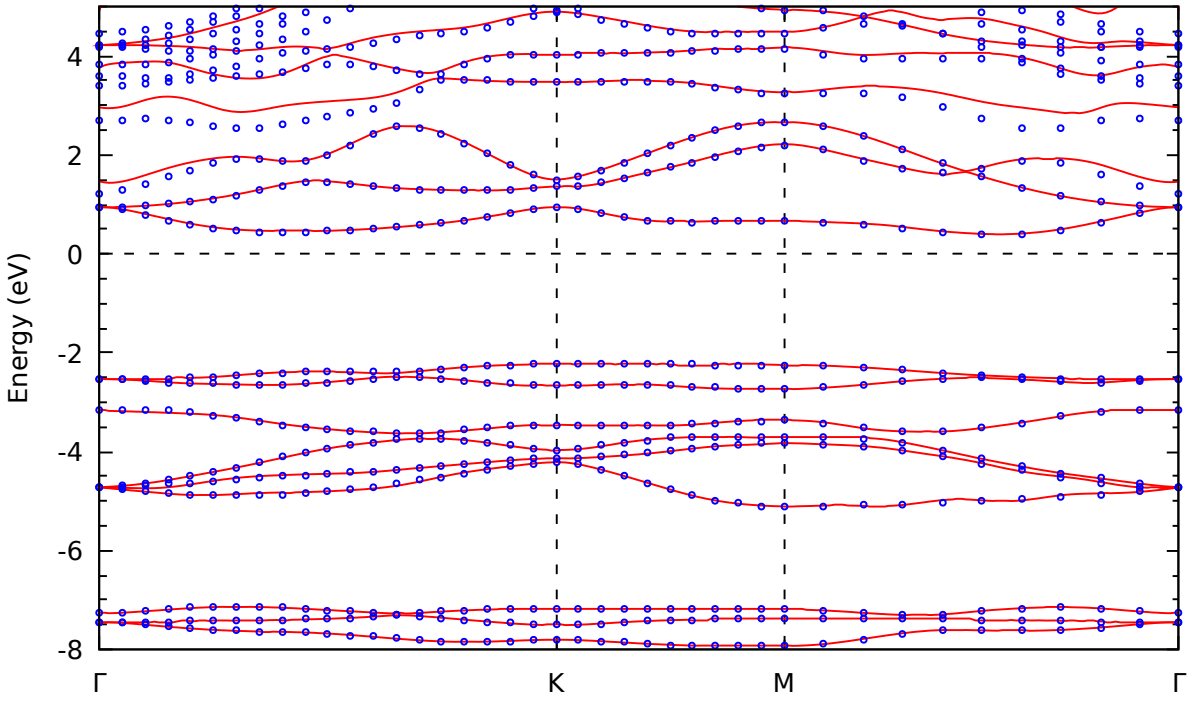

Figure S3 Disentangled band structure of YZrCOF monolayer. The solid red lines are disentangled bands interpolated along the path through the Brillouin zone using DLWFs. The blue solid points are from a non-SCF calculation in Quantum Espresso.

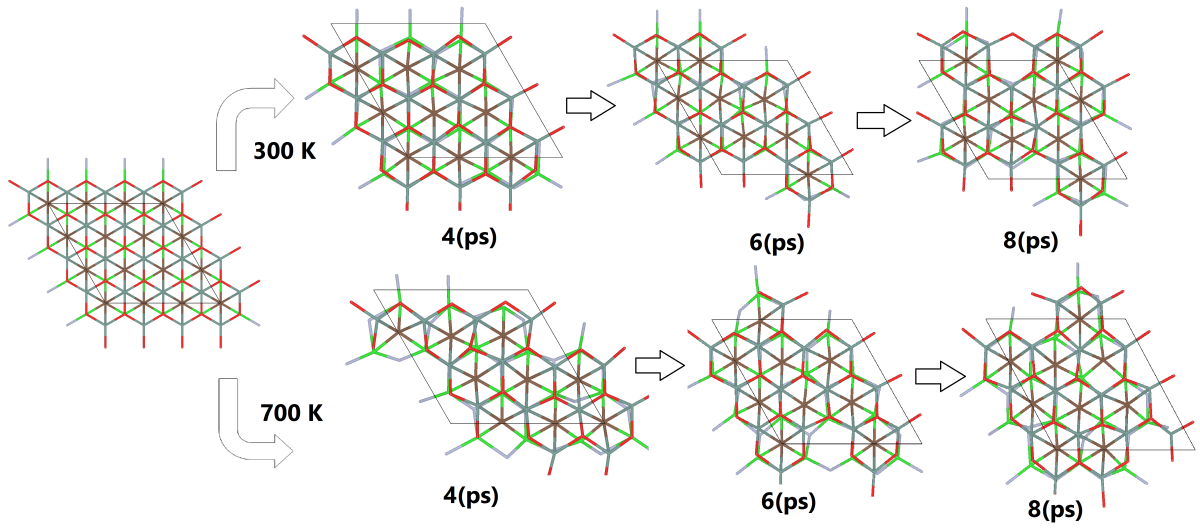

Figure S4 A representation of the YZrCOF supercells at different AIMD time steps. At the top, the structure for temperature equals 300, and at the bottom for 700 K

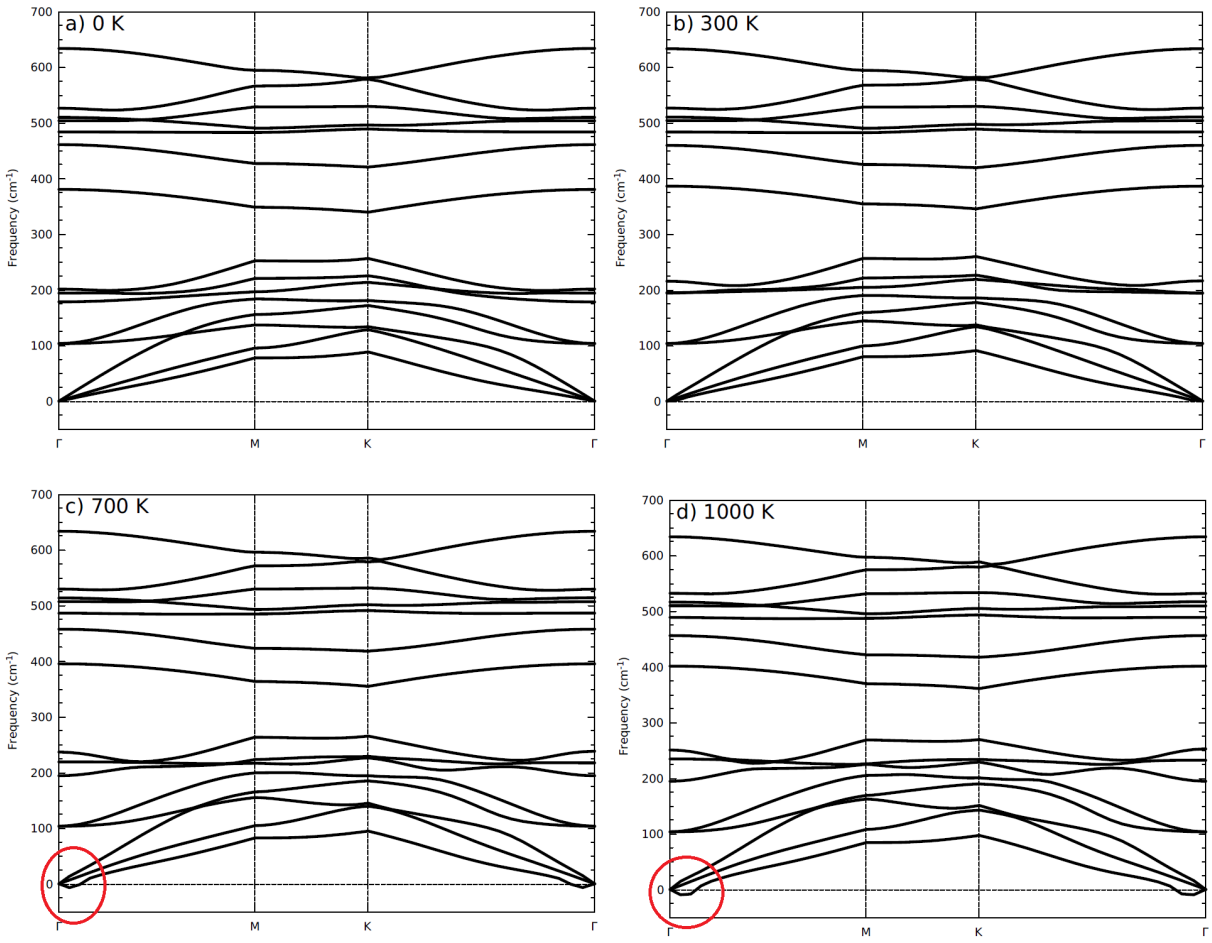

Figure S5 Anharmonic phonon dispersion curves of the YZrCOF monolayer as a function of temperature. The (a), (b), (c), and (d) plots correspond respectively to temperatures equal to 0, 300, 700, and 1000 K. The ALAMODE code[1] was used to simulate these curves using the finite displacement method. It is noted that at 1000 K the spectrum shows weak imaginary modes signature of dynamical instability.

References

(1) T. Tadano, Y. Gohda and S Tsuneyuki. Anharmonic force constants extracted from first-principles molecular dynamics: applications to heat transfer simulations. J. Phys.: Condens. Matter. **26** (2014) 225402. DOI: 10.1088/0953-8984/26/22/225402

(2) A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt, N. Marzari Wannier90: a tool for obtaining maximally-localized wannier functions Comput. Phys. Commun. **178** (2008) 685. https://doi.org/10.1016/j.cpc.2014.05.003